Elizabeth River PCB TMDL Study: Numerical Modeling Approach

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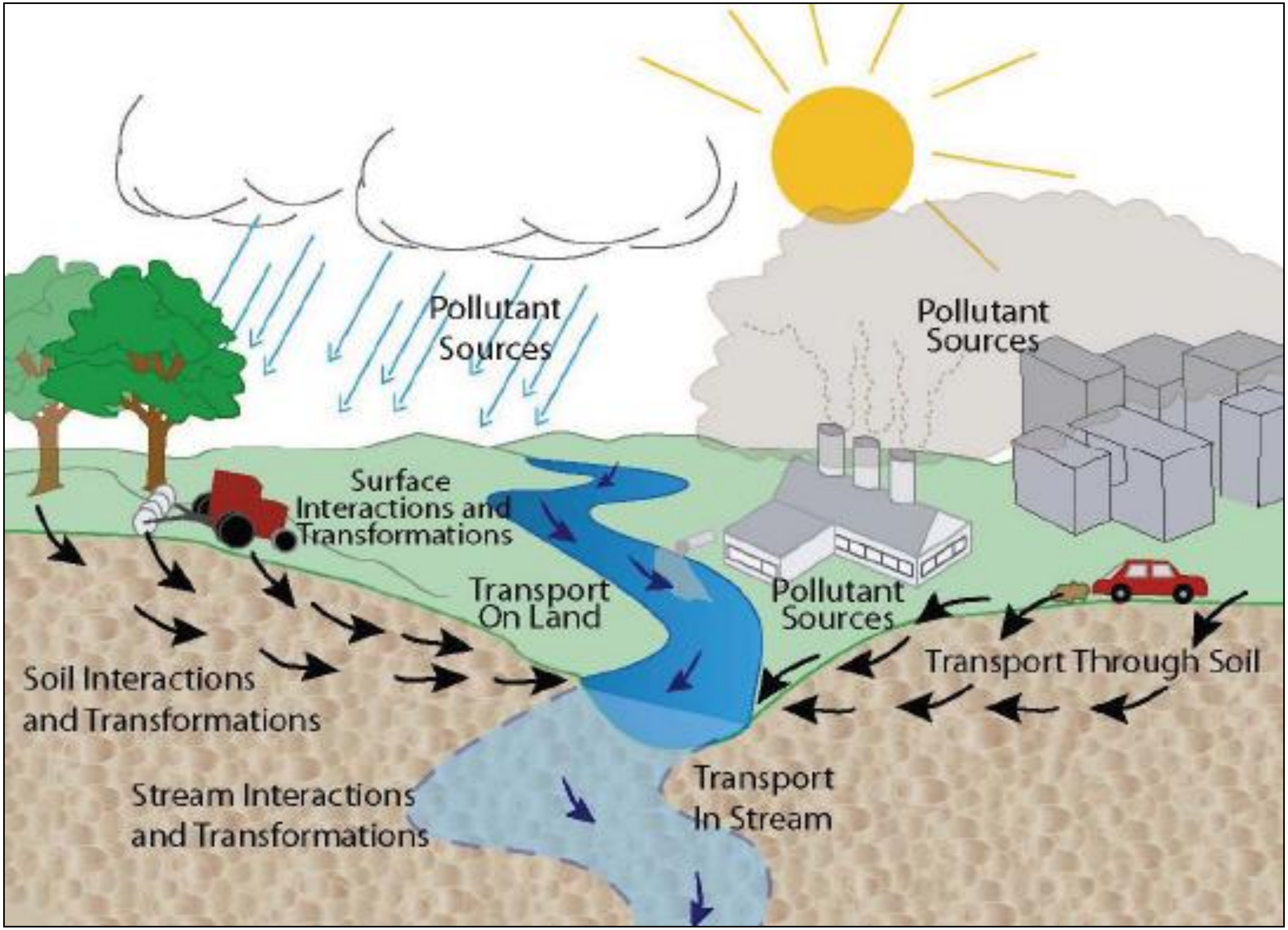
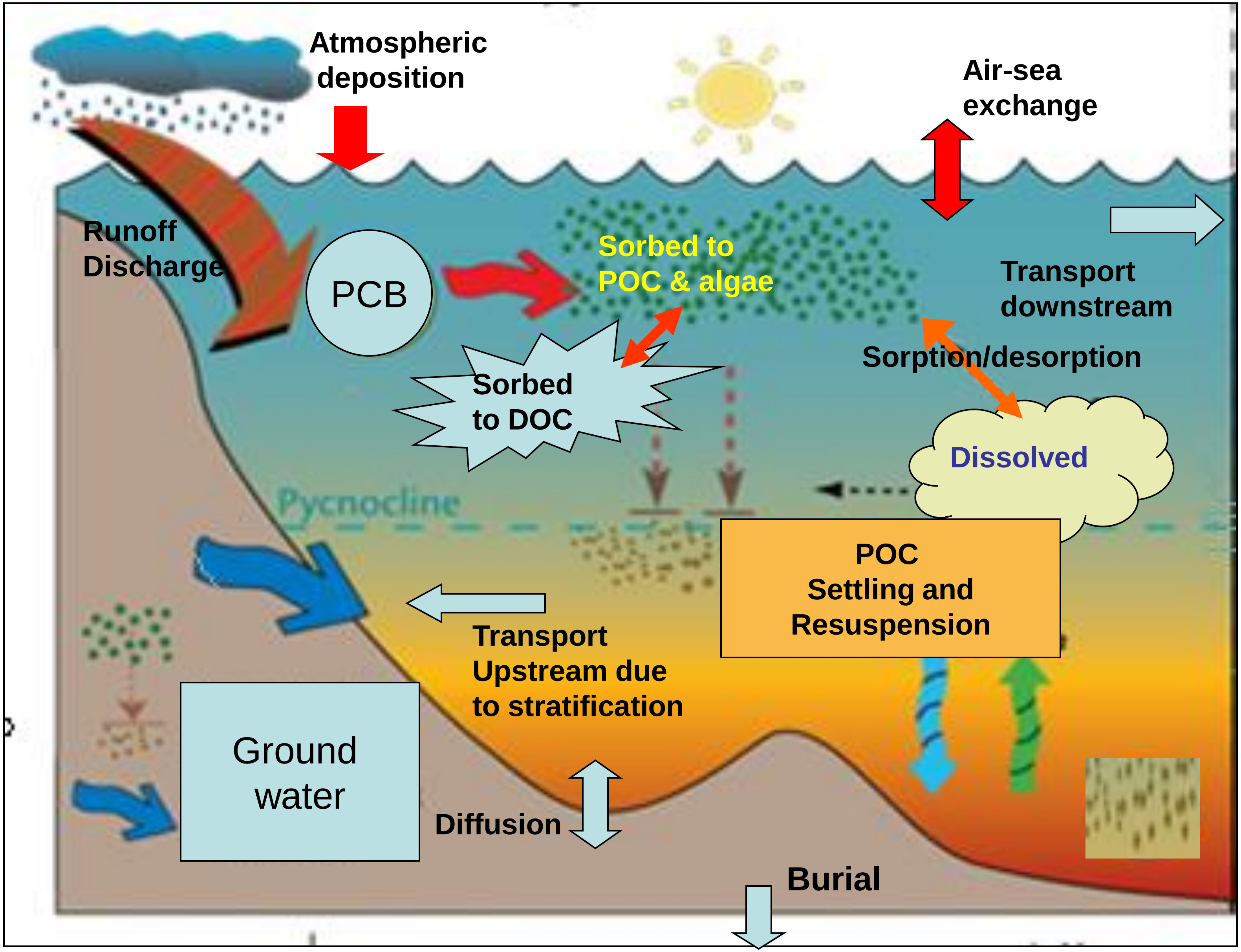
Pollutant Sources from Watershed

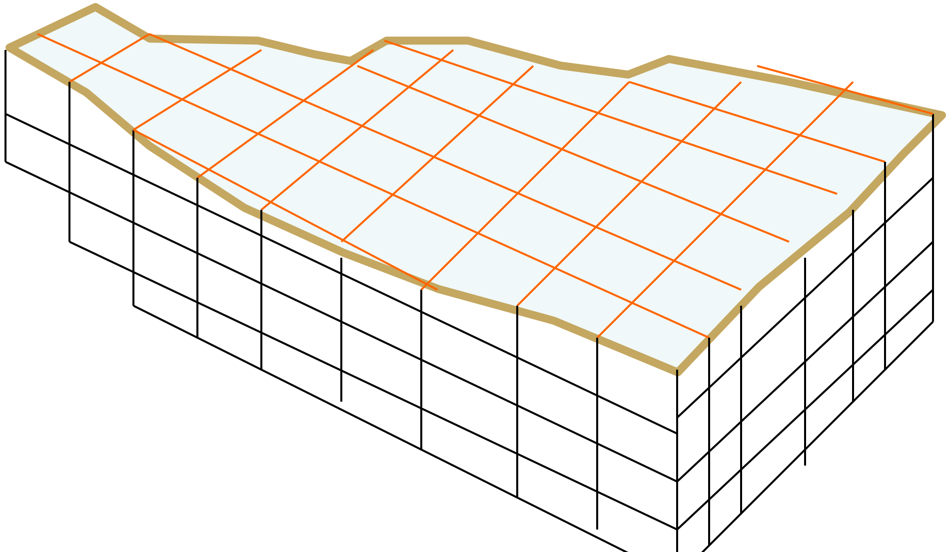


PCB Transport in Estuary

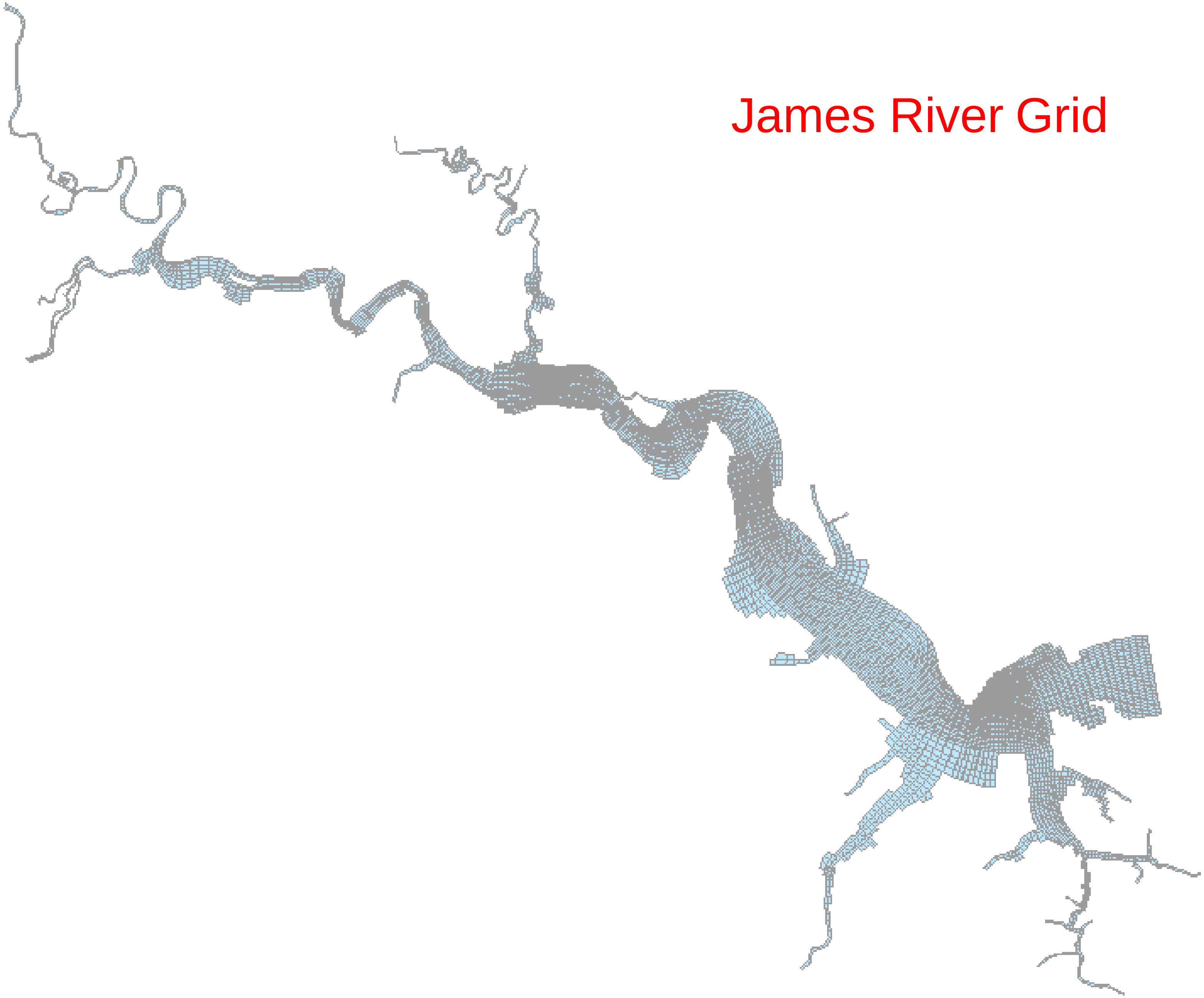


Modeling PCB concentrations in an Estuary

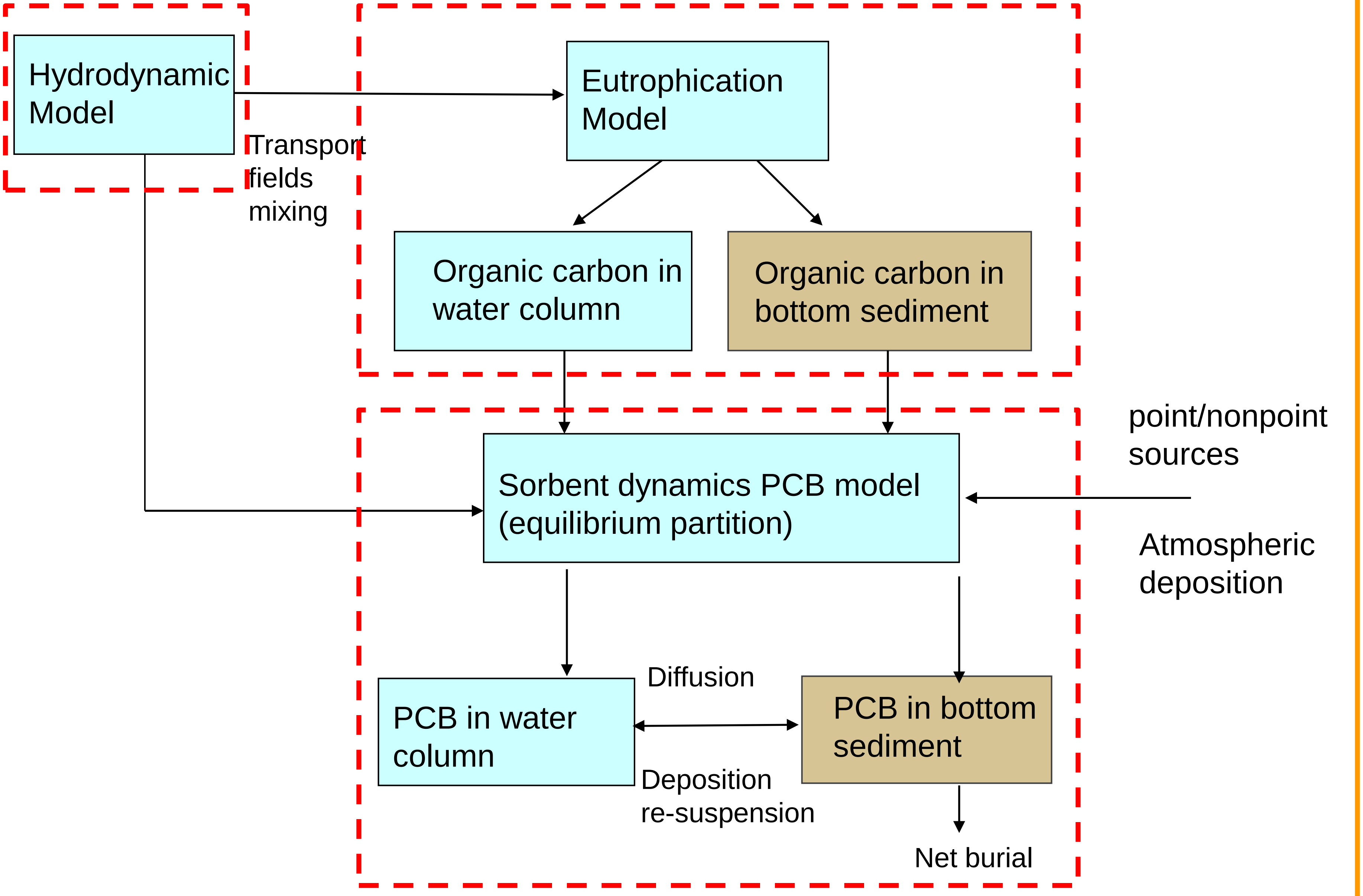
- Use environmental computer model to simulate PCB transport in the estuary
- Environmental computer models are mathematical representations of real-world conditions and are used to estimate environmental events and future changes.



James River Grid



Model Framework



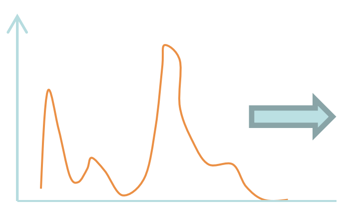
Hydrodynamic Model

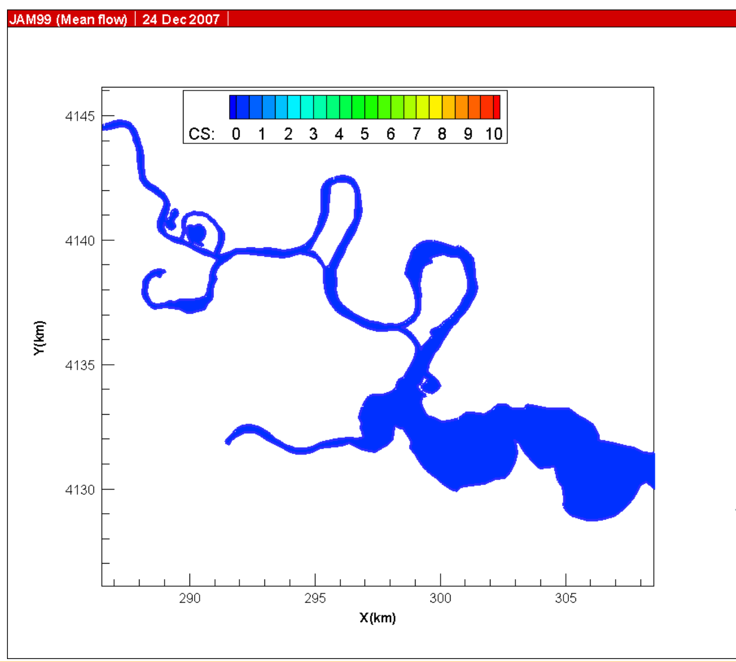
Tide, Temperature, Salinity, TSS, Meteorological forcing (wind, atm. pressure, dry & wet temperature, cloud cover, solar radiation)

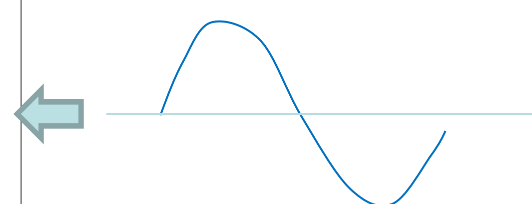
Surface elevation Current	Temperature	Salinity	Suspended sediment

Dynamic Model

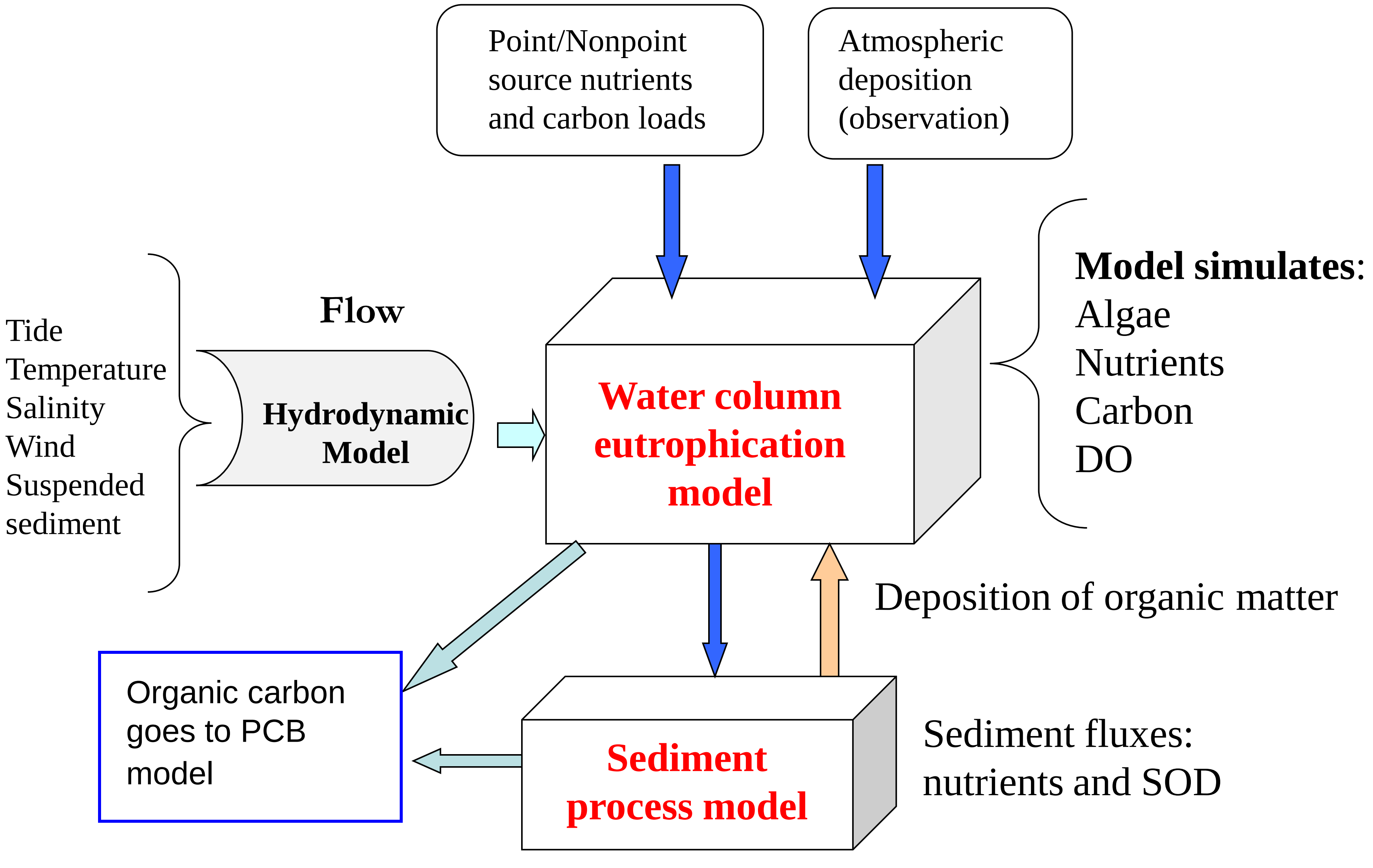
Provide transport fields for eutrophication and PCB models



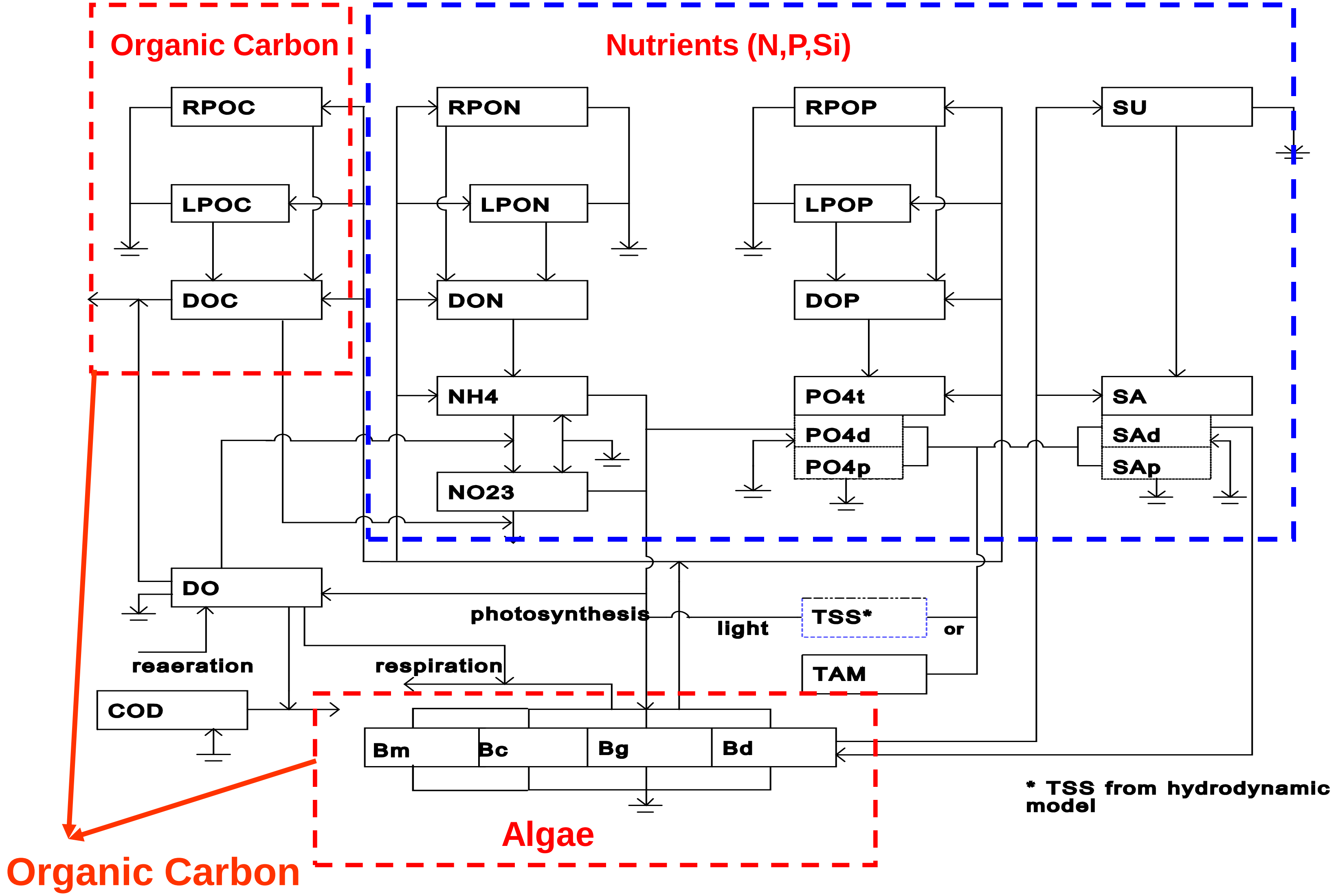




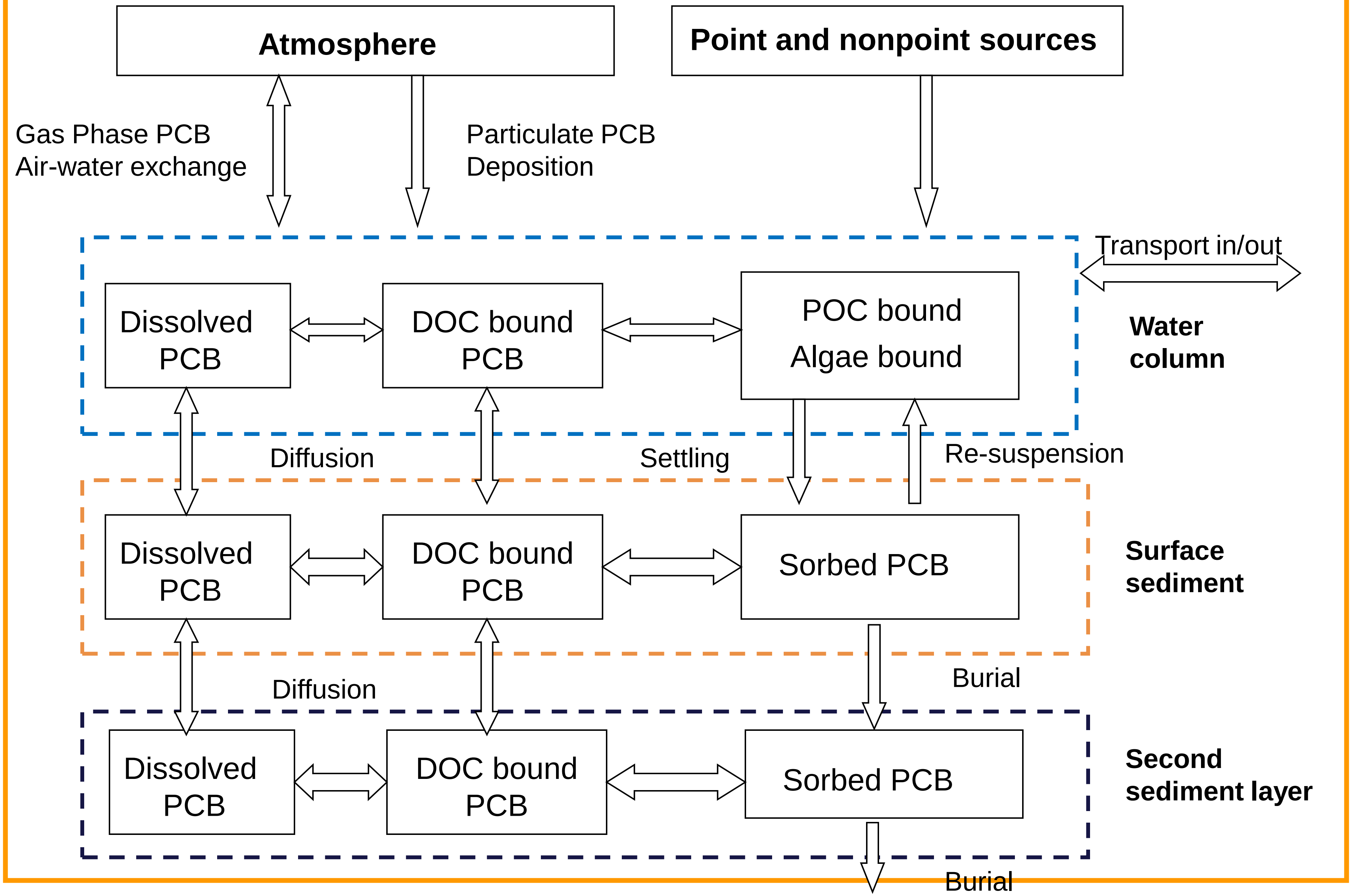
Eutrophication Model



Eutrophication (Organic carbon) Model

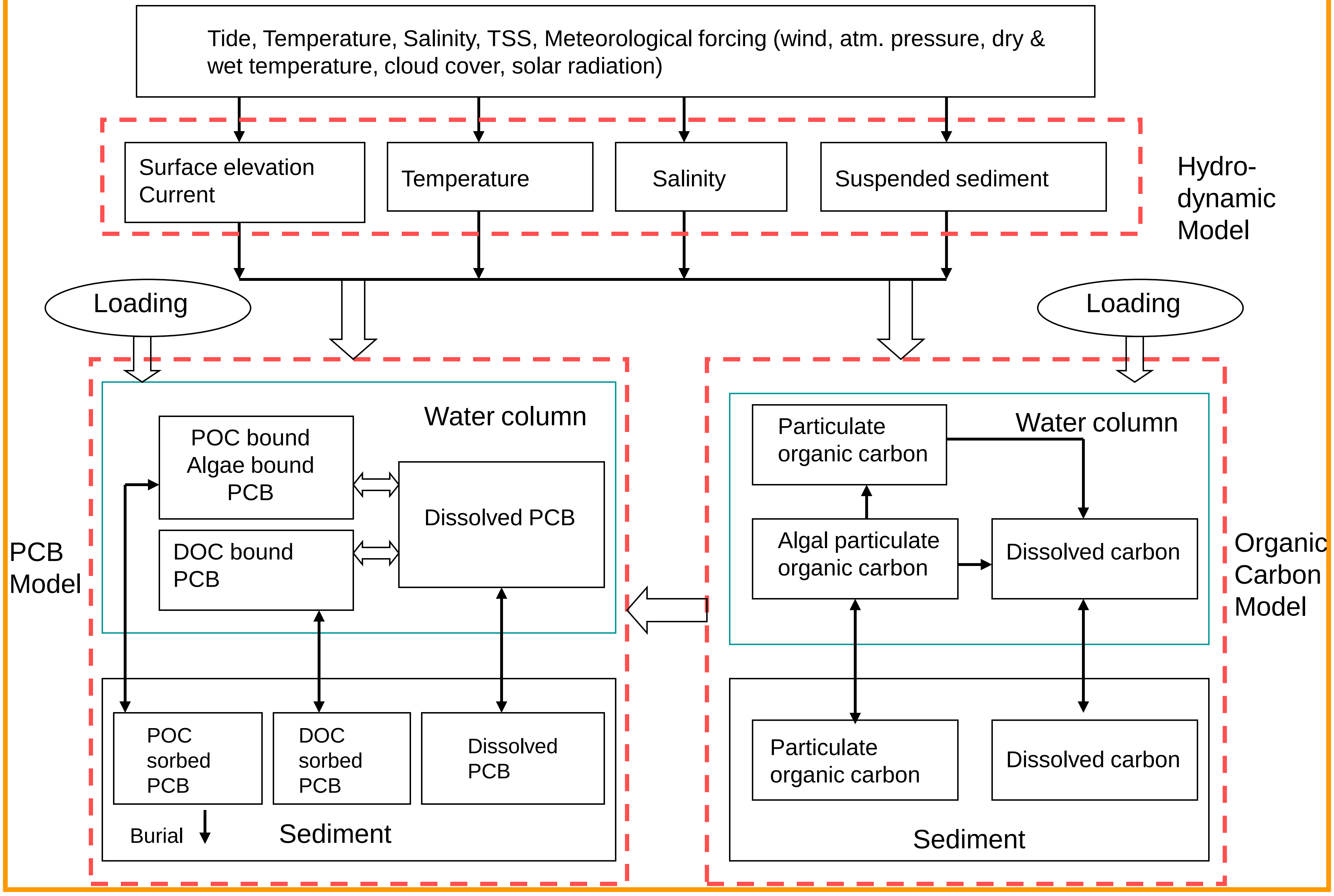


PCB Model

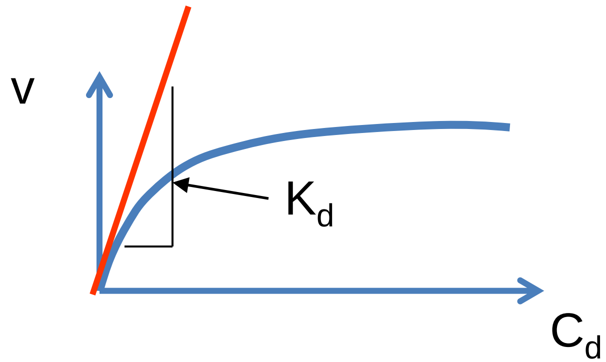


Atmosphere
Point and nonpoint sources
Gas Phase PCB
Air-water exchange
Particulate PCB
Deposition
Transport in/out
Dissolved PCB
DOC bound PCB
POC bound
Algae bound
Water column
Diffusion
Settling
Re-suspension
Dissolved PCB
DOC bound PCB
Sorbed PCB
Surface sediment
Diffusion
Burial
Dissolved PCB
DOC bound PCB
Sorbed PCB
Second sediment layer
Burial

Model Link Summary



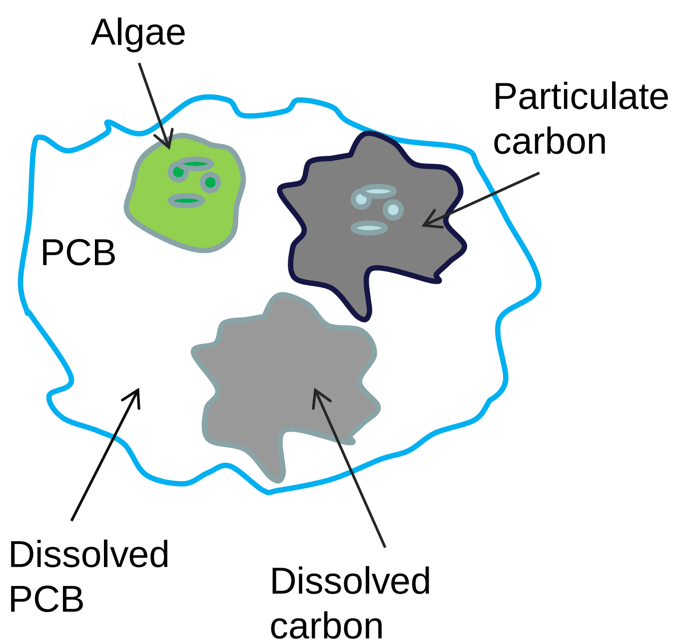
PCB Model Sorption Processes



v = PCB concentration on the solid / carbon (ng/g)
C_d =dissolved concentration (ng/L)

Equilibrium model assumes:

$$v = K_d \times C_d$$



The relationships between total PCB, dissolved PCB, particulate carbon bound PCB, algal bound PCB, and dissolved carbon bound PCB are:

Dissolved PCB (C_w):	$C_w = f_w \times C$
Particulate Carbon pound PCB (C_P^1):	$C_P^1 = f_P^1 \times C$
Algae bound PCB (C_P^2):	$C_P^2 = f_P^2 \times C$
Dissolved organic carbon bound PCB (C_D):	$C_D = f_D \times C$

f_x = fraction of each component
C = total PCB

$$f_w + \sum_i f_P^i + f_D = 1 \qquad (1)$$

$$fw = \frac{Cw}{C} = \frac{\phi}{\phi + \sum_i K_P^i m_P^i + K_D m_D} \qquad (2)$$

$$f_P^i = \frac{C_P^i}{C} = \frac{K_P^i m_P^i}{\phi + \sum_i K_P^i m_P^i + K_D m_D} \qquad (3)$$

$$f_D = \frac{C_D}{C} = \frac{K_D m_D}{\phi + \sum_i K_P^i m_P^i + K_D m_D} \qquad (4)$$

Where m_P^1, m_P^2, m_D are particulate organic carbon, particulate algal carbon, and dissolved organic carbon. K_P^1, K_P^2, and K_D denote the partition coefficients, respectively for three carbon species.

Dissolved PCB (C_w):	$C_w = f_w \times C$
Particulate Carbon pound PCB (C_P^1):	$C_P^1 = f_P^1 \times C$
Algae bound PCB (C_P^2):	$C_P^2 = f_P^2 \times C$
Dissolved organic carbon bound PCB (C_D):	$C_D = f_D \times C$

PCB Transport Model Equation

$$\partial_t \left(m_x m_y H C\right) + \underbrace{\frac{1}{m_x m_y}\partial_x \left(m_y H u C\right) + \frac{1}{m_x m_y}\partial_y \left(m_x H v C\right) + \partial_x \left(m_x m_y w C\right)}_{\text{Transport}}$$

$$-\partial_x \underbrace{\left(m_x m_y \sum_i w_s^i f_p^i C \right)}_{\text{Settling}} = \partial_z \underbrace{\left(m_x m_y \frac{A_b}{H} \partial_z C \right)}_{\text{Diffusion}} - \left(m_x m_y H \gamma C\right)$$

Where *H* is water depth, C is total PCB concentration, A_b is eddy diffusivity, and w_s^i (i=1,2) are settling velocities associated with particulate organic carbon and algal organic carbon, γ is decay constant, *u*, *v*, *w* are velocity at x-, y-, and z- directions, m_x and m_y are scale factors of the horizontal coordinates.

The boundary condition at the water column sediment interface, z = 0, is:

$$-\frac{A_b}{H}\partial_z C - \sum_i w_s^i f_s^i C =$$

$$= \sum_i \left[\max \left(\frac{J_P^i f_P^i}{m_P^i}, 0 \right) C \right]_S + \sum_i \left[\min \left(\frac{J_P^i f_P^i}{m_P^i}, 0 \right) C \right]_W - q_{dif} \left(\frac{f_w + f_D}{\phi} C \right)_W + q_{dif} \left(\frac{f_w + f_D}{\phi_s} C \right)_S$$

Where J_P^i (i=1,2) are POC and algal carbon fluxes between sediment bed, and water column (mass per unit area per second), defined as positive from the bed, ϕ and ϕ_s are porosities in water column and sediment. The subscripts 'w' and 's' denote water column and sediment, respectively, and q_{dif} is diffusion velocity.

The volatilization which occurs at the surface depends on the mass transfer coefficient at the air-water interface and the concentration of PCB in the water column. The boundary condition at the water column and air interface, z = 1, is:
(Bamford, et al., 2002)

$$-\frac{A_b}{H}\partial_z C - \sum_i w_s^i f_s^i C = \frac{K_V}{\Delta Z}\left[f_w C - \frac{C_a}{K_{H'}} \right]$$

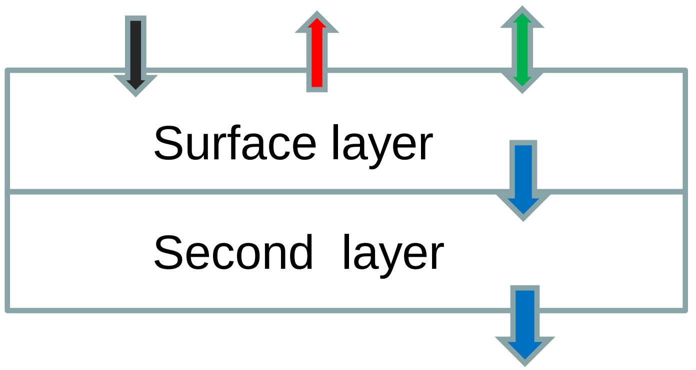
Where K_v is the volatilization mass transfer coefficient (L/T), ΔZ is the thickness of the first layer near the surface, C_a is the vapor phase PCB concentration in air (M/L^3) and K_H is the dimensionless, temperature-corrected Henry's law constant.

Bottom Sediment Model Equation

$$\partial_t (BC)_T = -\gamma (BC)_T$$

$$-\sum_i \left[\underbrace{\max \left(\frac{J_P^i f_P^i}{B m_P^i}, 0 \right)}_{\text{Lost due to re-suspension}} BC \right]_{T+} - \sum_i \left[\underbrace{\min \left(\frac{J_P^i f_P^i}{m_P^i}, 0 \right)}_{\text{Settling from water column}} C \right]_W - \sum_i \left[\underbrace{\min \left(\frac{J_P^i f_P^i}{B m_P^i}, 0 \right)}_{\text{Settling to deep sediment layer}} BC \right]_{T-}$$

$$\underbrace{+ q_{dif} \left(\frac{f_w + f_D}{\phi} C \right)_W - q_{dif} \left(\frac{f_w + f_D}{\phi_s} C \right)_T}_{\text{Diffusion between water column and sediment}}$$

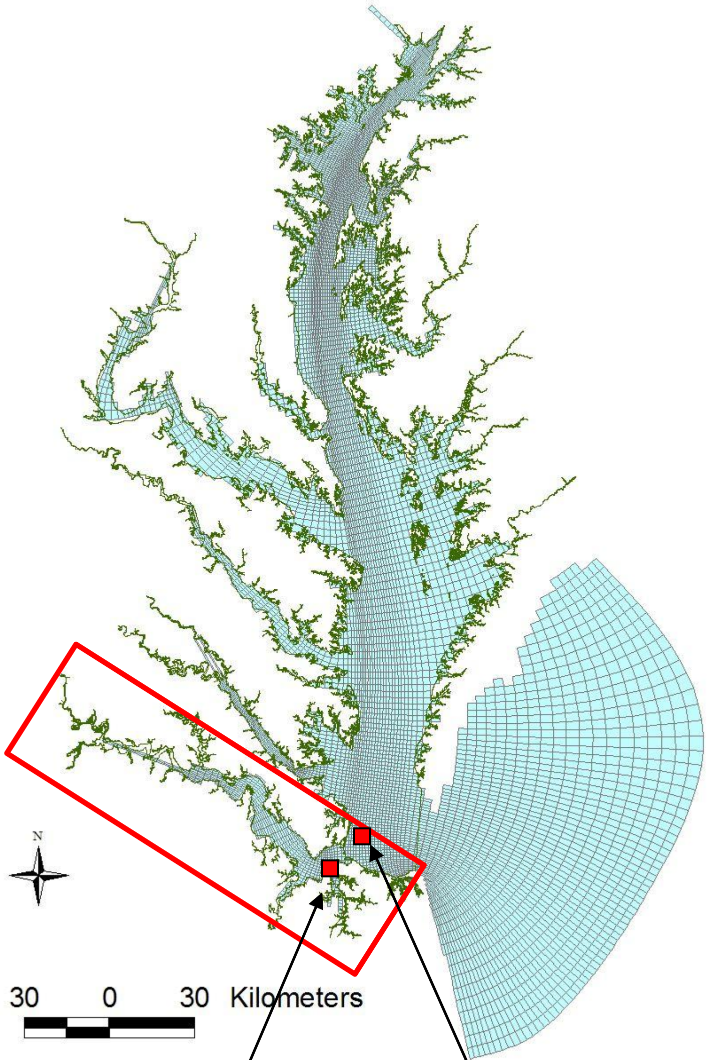


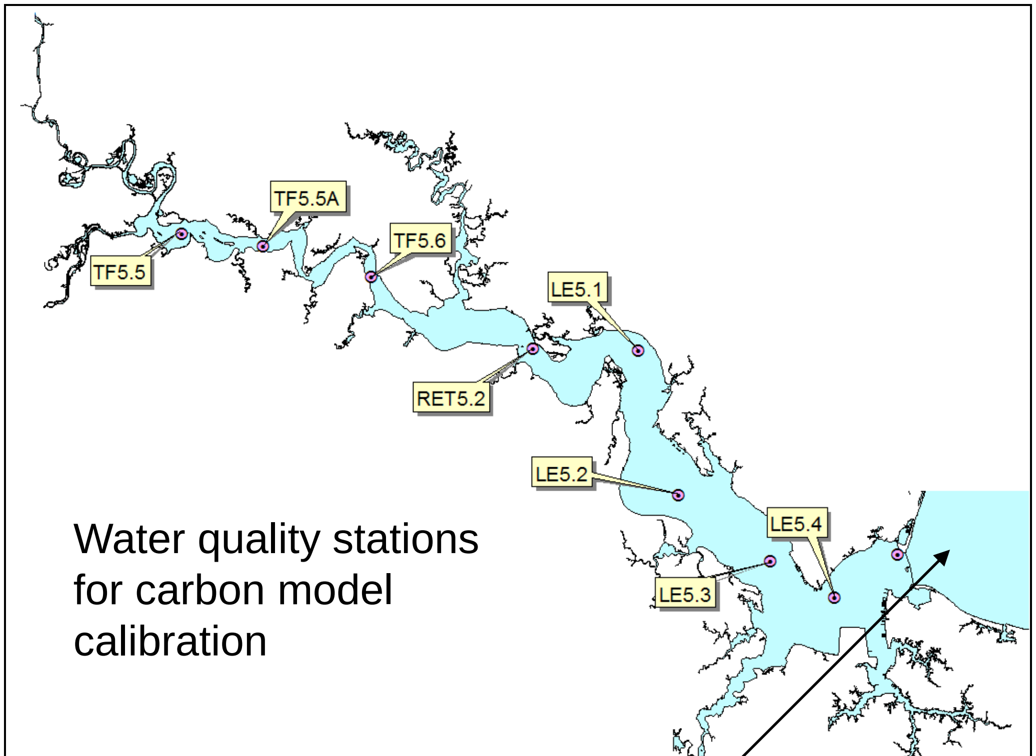
Where B is the thickness of the sediment layer.

Data Needed for Hydrodynamic Model Calibration

- Tide
  - use NOAA observation data at Sewells Point
- Salinity at open boundary
  - use the Chesapeake Bay model output (available from 1997-2007)
- Flow data
  - use USGS upstream daily flow (Appomattox River USGS02041650 and Richmond station USGS37500)
- Meteorological forcing data
  - use NOAA data at Sewells and Gloucester Point
    - wind, atmospheric pressure
    - dry & wet temperature
    - cloud cover and solar radiation

Link James River Model to the Bay Model



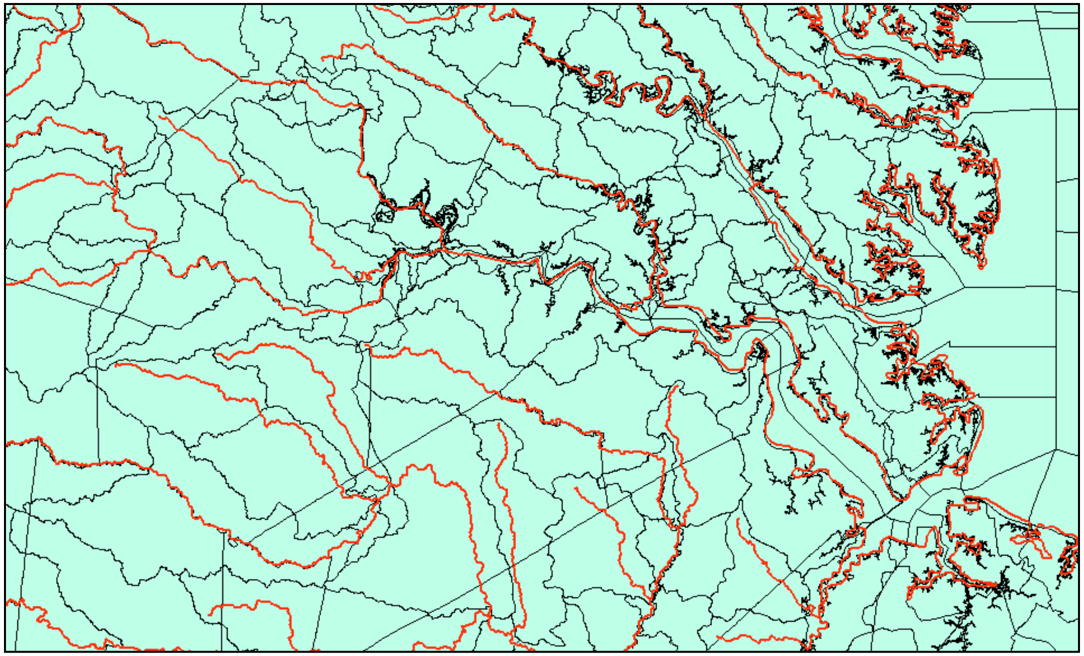


Sewells Point

Output salinity will be used for James River model boundary condition at the mouth

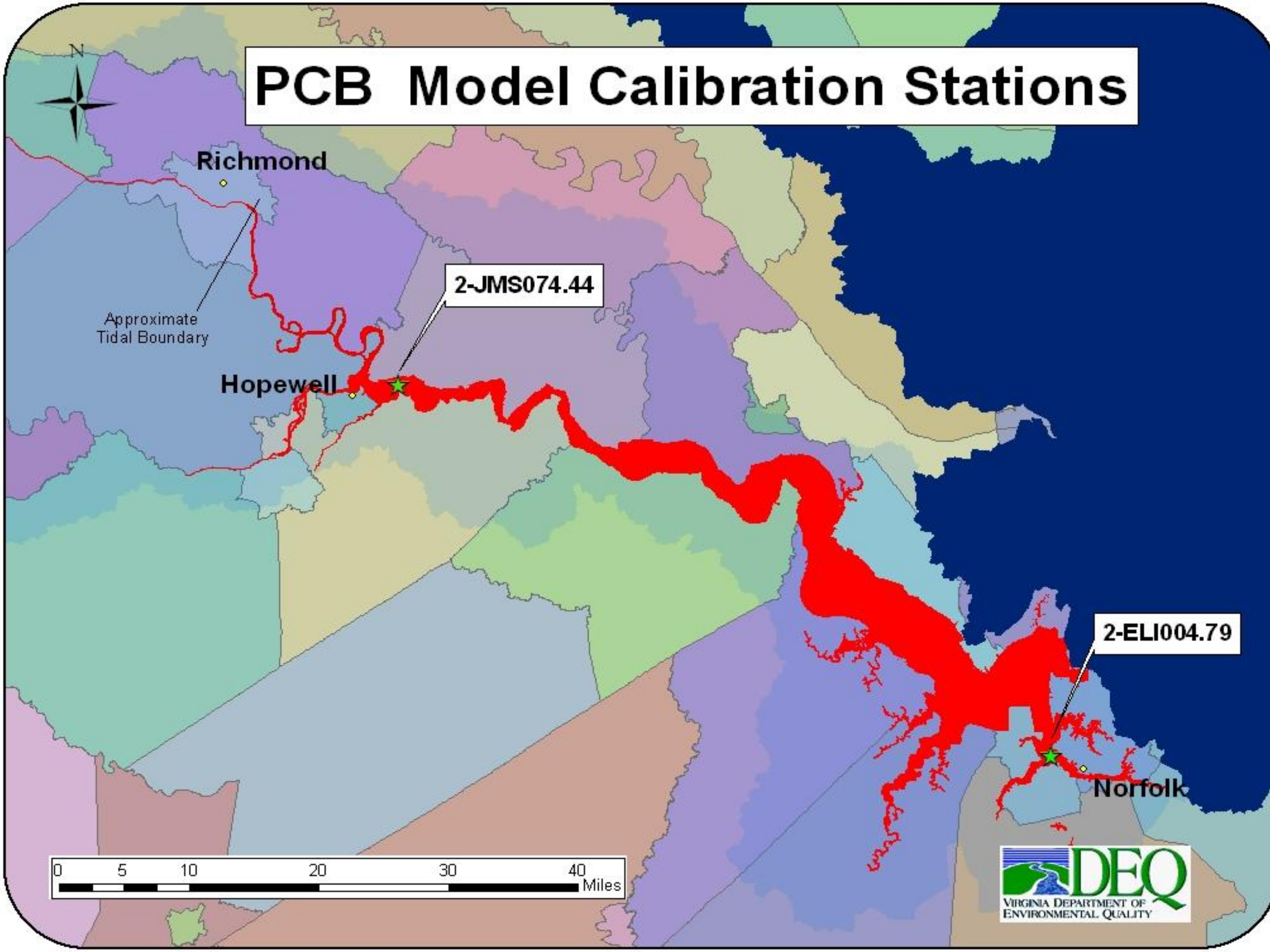
Data Needed for Eutrophication Model Calibration

- Point source loading
  - Chesapeake Bay program/DEQ
- James River mouth open boundary
  - Monthly observations
- Nonpoint source loading
  - Chesapeake Bay Phase V watershed model output, 1980-2005
    - Flow
    - Nitrogen
    - Phosphorus
    - Carbon
    - Algae



Data Needed for PCB Model Calibration

- Bottom sediment PCB data
  - use for initial sediment condition (sediment study)
- Upstream PCB data
  - estimate upstream PCB inflow
- Loading from contaminated sides
- Storm water data ?
- Point source data ?
- Nonpoint source loading (background, unknown loadings)
  - estimate based on event driven concentration and flow
- Atmospheric deposition
  - Historical observations/new observations
- Model calibration data
  - Collect short-term data covering large area
  - Intensive survey data
    - monthly or bimonthly PCB data for a year at 2-3 stations (i.e., 2-JMS074.44, 2-ELI04.79)


PCB Model Calibration Stations
N
Richmond
Approximate
Tidal Boundary
2-JMS074.44
Hopewell
2-ELI004.79
Norfolk
0 5 10 20 30 40
Miles
DEQ
Virginia Department of
Environmental Quality

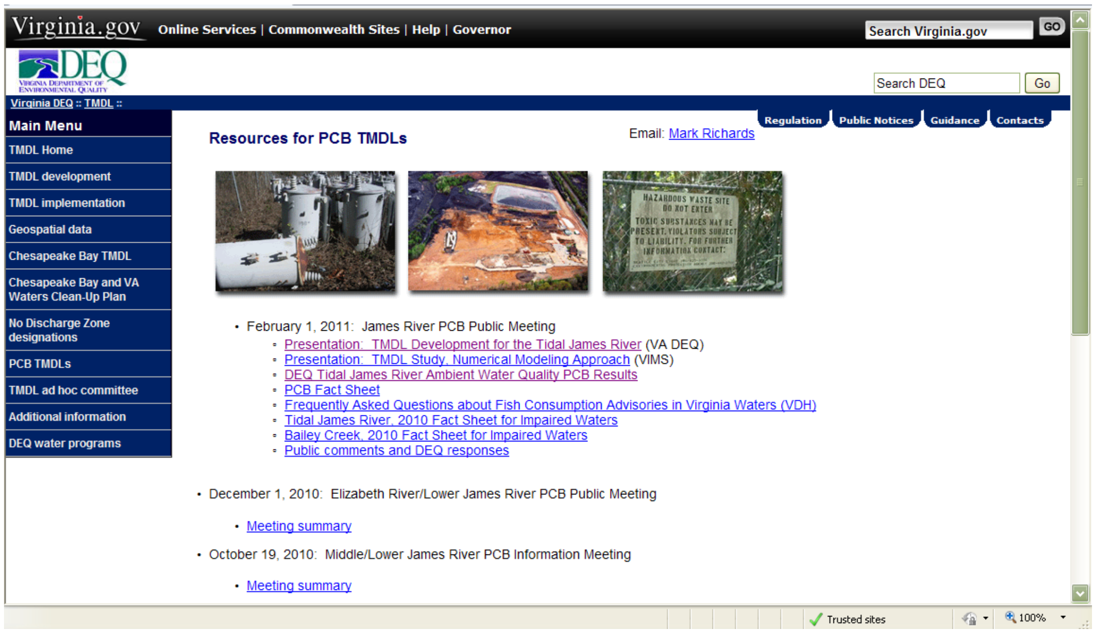
Next Steps…

- Data collection
- Nonpoint source estimation
- Pollutant source estimation
- Model setup
- Hydrodynamic model calibration
- Eutrophication model calibration
- PCB Model calibration procedure

Questions / Discussion

DEQ PCB TMDL website:

http://www.deq.virginia.gov/tmdl/pcb.html



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